Surface Fluxes, Implicit Time Stepping, and the Exchange Grid: The Structure of the Surface Exchange Module

October 4, 2004

The computation of surface fluxes over land and ice raises a variety of issues with regard to the exchange grid and the implicit treatment of fluxes within the atmosphere and within the land and ice models. Criteria that help us choose between alternative schemes are
• Conservation: the quantity transported across the surface must be conserved;
• Stability: the scheme should be as stable as possible and free of unphysical oscillations so that the flux computation itself does not introduce any limitations on model time steps. In particular, one should be able to take the limit of inifinitesimal land heat capacity, or very high vertical resolution near the surface in the atmosphere;
• Modularity: the land, ice, and atmosphere models should be unaware of the grids being used by the other models in the system.

1 A starting point

Consider the following simple model, in which we will assume that the atmospheric and land grids are identical for the time being.

$$c_A \partial T_A / \partial t = F(T_A, T_L) \tag{1}$$

$$c_L \partial T_L / \partial t = -F(T_A, T_L) \tag{2}$$

The atmosphere and the land exchange the heat flux F. As the simplest case, set $F(T_A, T_L) = -\gamma(T_A - T_L)$. In the uncoupled case ($T_L =$constant) the simplest forward time step is

$$c_A \frac{(T_A^{i+1} - T_A^i)}{\Delta t} = -\gamma T_A^i \tag{3}$$

which blows up if $\xi_A > 2$ and produces oscillatory rather than monotonic decay for $1 < \xi_A < 2$, where $\xi_A \equiv \gamma \Delta t / c_A$. This is unacceptable. A centered step, with $0.5\gamma(T_A^{i+1} + T_A^i)$ on the RHS, is stable in the sense that all solutions are damped, but when $\xi_A > 2$ it produces oscillatory decay, which is still unacceptable. The standard procedure is to use a backward time step

$$c_A \frac{(T_A^{i+1} - T_A^i)}{\Delta t} = -\gamma T_A^{i+1} \tag{4}$$

which is stable and decays monotonically in all cases. (In fact, in some atmospheric models, the surface fluxes are computed with a "super backwards" scheme, in which, on the RHS, $T_A \rightarrow \alpha T_A^{i+1} + (1-\alpha)T_A^i$, with $\alpha > 1$)

The same argument holds for the coupled system, (1) and (2). The fully explicit forward scheme is unstable for either large ξ_A or ξ_L, where $\xi_L \equiv \gamma\Delta t/c_L$, and the 'half' explicit schemes $F(T_A^{i+1}, T_L^i), F(T_A^i, T_L^{i+1})$ also do not allow arbitrary time steps or heat capacities. The fully implicit scheme $F(T_A^{i+1}, T_L^{i+1})$ is the preferred choice.

(If conservation were not a requirement, other options would be available, such as

$$c_A \frac{(T_A^{i+1} - T_A^i)}{\Delta t} == F(T_A^{i+1}, T_L^i) \tag{5}$$

$$c_L \frac{(T_L^{i+1} - T_L^i)}{\Delta t} = -F(T_A^{i+1}, T_L^{i+1}) \tag{6}$$

which has the advantage of decoupling the two equations. We require the FMS flux exchange module to conserve exactly, ruling out such options.)

Returning to a general expression for $F(T_A^{i+1}, T_L^{i+1})$, we replace it by the first term in its Taylor expansion about its value F_0 at the time step i:

$$\frac{c_A}{\Delta t}\Delta T_A = F_0 + \frac{\partial F}{\partial T_A}\Delta T_A + \frac{\partial F}{\partial T_L}\Delta T_L \tag{7}$$

$$\frac{c_L}{\Delta t}\Delta T_L = -F_0 - \frac{\partial F}{\partial T_A}\Delta T_A - \frac{\partial F}{\partial T_L}\Delta T_L \tag{8}$$

where $\Delta T \equiv T^{i+1} - T^i$. Note that this linearization does not destroy exact energy conservation; we have simply modified the form of the exchanged flux slightly. The linearization is a device to avoid iterating for the implicit solution. Once one has chosen a backwards scheme, the iterated solution is, in general, no more accurate than the solution with linearized fluxes. The only disadvantage of the latter is a "diagnostic" one: the fluxes exchanged between the two models cannot be considered precisely as a function F of atmospheric and land states at particular times; they are also a function of the change in state from one time step to the next.

We now have two equations that can be solved simultaneously for the two unknowns ΔT_A and ΔT_L. This is straightforward, of course, but we would like to formulate things so that the two models remain as modular as possible, without being unnecesarily intertwined. For this purpose, it is useful to think of first solving the atmospheric equation, which provides ΔT_A as a (linear) function of ΔT_L.

$$\Delta T_A = e\Delta T_L + f \tag{9}$$

In this case

$$f \equiv \Gamma F_0 \tag{10}$$

and

$$e \equiv \Gamma \frac{\partial F}{\partial T_L} \tag{11}$$

where

$$\Gamma \equiv (\frac{c_A}{\Delta t} - \frac{\partial F}{\partial T_A})^{-1} \tag{12}$$

Using this linear relation, ΔT_A can be eliminated and the land model can be recast into the form

$$\frac{c_L}{\Delta t}\Delta T_L = -(\alpha + \beta \Delta T_L) \tag{13}$$

which is then easily solved for ΔT_L. Here

$$\alpha \equiv F_0 + \frac{\partial F}{\partial T_A} f \tag{14}$$

$$\beta \equiv \frac{\partial F}{\partial T_L} + \frac{\partial F}{\partial T_A} e \tag{15}$$

Once ΔT_L is known we can return to (9) and compute ΔT_A

To summarize this procedure –

• Compute

$$F_0, \frac{\partial F}{\partial T_A}, \frac{\partial F}{\partial T_L} \tag{16}$$

• compute e and f, and then α and β.

•ask the surface model(s) to compute the change in surface temperature, given a flux of the form $\alpha + \beta \Delta T_L$

• given this change in the surface temperature, ask the atmosphere to update the atmospheric temperature using (9).

2 Implicit fluxes within the atmosphere

We need several generalization of this procedure for the flux exchange module in FMS. We first interpret T_A as referring to the "lowest atmospheric model layer". (In the simplest energy balance atmospheric models, this layer could be the entire atmosphere.) We now need to leave open the possibility that there are atmospheric fluxes into this atmospheric box from above that are treated implicitly.

When there are two distinct processes in a model that must both be treated implicitly, it is not necessarily a requirement that the implicit computations be coupled. One can instead use some time-splitting procedure in which one computes the effects of process A as if process B were not present or in which B is treated explicitly, then uses the resulting state of the system as input into an implicit computation of the effects of B.

In a GCM the vertical diffusive fluxes are generally treated implicitly; furthermore, the diffusive flux across the top of the lowest atmospheric grid box can be closely related to the surface flux, especially when this lowest atmospheric box is very thin. (Quite often we pretend that the lowest atmospheric layer lies completely within the "constant flux layer" within the atmospheric turbulent boundary layer, so as to justify the use of Monin-Obukhov similarity theory, in which case the diffusive flux at the top of the lowest layer should be essentially the same as the surface flux.) Therefore, not only is it desirable to treat the vertical diffusion within the planetary boundary layer implicitly, but we need to treat the surface fluxes and the vertical diffusive fluxes near the surface as part of the *same* implicit step.

Consider, therefore,

$$c_A \partial T_A / \partial t = F(T_A, T_L) + F_A(T_A, \xi_A) \tag{17}$$

where F_A is a flux into the box from above which depends on T_A and other atmospheric variables ξ_A (for the most relevant example of a local diffusive flux, ξ_A is the temperature at the level above the lowest model level). Evaluate all variables on the RHS at $t = i + 1$, and proceed with a linear Taylor expansion as above. The flux F_A is now approximated by

$$F_A(T_A, \xi_A) = F_A(T_A^i, \xi_A^i) + \frac{\partial F_A}{\partial T_A} \Delta T_A + \frac{\partial F_A}{\partial \xi_A} \Delta \xi_A \tag{18}$$

We now need to assume the existence of a precomputation within the atmospheric model which relates $\Delta\xi_A$ to ΔT_A:

$$\Delta\xi_A = e_A \Delta T_A + f_A \tag{19}$$

with the result

$$F_A(T_A, \xi_A) = (F_A)_0 + \frac{dF_A}{dT_A}\Delta T_A \tag{20}$$

where

$$\frac{dF_A}{dT_A} \equiv \frac{\partial F_A}{\partial T_A} + e_A \frac{\partial F_A}{\partial \xi_A} \tag{21}$$

$$(F_A)_0 \equiv F_A(T_A^i, \xi_A^i) + f_A \frac{\partial F_A}{\partial \xi_A} \tag{22}$$

We can now solve our coupled atmosphere-land system exactly as before by modifying the definion of Γ:

$$\Gamma \equiv (\frac{c_A}{\Delta t} - \frac{\partial F}{\partial T_A} - \frac{dF_A}{dT_A})^{-1} \tag{23}$$

and replacing F_0 by $F_0 + (F_A)_0$

For the relevant case of vertical diffusion, the atmospheric precomputation is easily accomplished. The tridiagonal matrix that results from the implicit diffusion operator is most efficiently solved by a standard two-sweep algorithm. Starting at the top of the atmosphere, one uses the matrix elements to recursively generate the coefficients e_k and f_k that one can then use to generate the temperature increments in an upeward recursive sweep of an equation of the form

$$\Delta T_{k-1} = e_k \Delta T_k + f_k \tag{24}$$

where the index k increases downwards. If the last grid box is $k = N$, then e_N and f_N play the role of e_A and f_A above. The flux exchange module does not need to know the details of this computation; it only requires the resulting modified flux and derivative defined by (21) and (22).

3 Leapfrog

We also need to allow for the possibility that the atmosphere is integrated with a leapfrog step and the land with a forward step – a common combination in practice. We then have, leaving F_A out for simplicity,

$$c_A \frac{T_A^{i+1} - T_A^{i-1}}{2\Delta t} = F(T_A^{i+1}, T_L^{i+1}) \tag{25}$$

$$c_L \frac{T_L^{i+1} - T_L^{i}}{\Delta t} = F(T_A^{i+1}, T_L^{i+1}) \tag{26}$$

Energy will still be conserved every two time steps in the sense that

$$c_A \frac{T_A^{i+2} + T_A^{i+1}}{2} + c_L T_L^{i+2} = c_A \frac{T_A^{i} + T_A^{i-1}}{2} + c_L T_L^{i} \tag{27}$$

We now expand F about the temperatures T_A^{i-1} and T_L^i

$$F(T_A^{i+1}, T_L^{i+1}) \approx F(T_A^{i-1}, T_L^{i}) + \frac{\partial F}{\partial T_A}\Delta T_A + \frac{\partial F}{\partial T_L}\Delta T_L \tag{28}$$

where now

$$\Delta T_A \equiv T_A^{i+1} - T_A^{i-1} \tag{29}$$

$$\Delta T_L \equiv T_L^{i+1} - T_L^{i} \tag{30}$$

The rest of the derivation proceeds exactly as before. We need only be careful that $2\Delta t$ is substituted for Δt in the expression for Γ.

4 Evaporation

Now consider the case in which we have evaporation as well as sensible heat flux. The evaporation E, might be a function of a variety of things, but the only functional dependence we are concerned with is that part that is treated implicitly. In the current implementation of FMS (Eugene) E as an implicit function of q_A, the specific humidity in the atmosphere, and T_L, the surface temperature.

$$c_A \partial T_A / \partial t = F(T_A, T_L) \tag{31}$$

$$\partial q_A/\partial t = E(q_A, T_L) \tag{32}$$

$$c_L \partial T_L/\partial t = -F(T_A, T_L) - LE(q_A, T_L) \tag{33}$$

After a Taylor's expansion as above, we can solve the atmospheric equation for ΔT_A as a function of ΔT_L as before:

$$\Delta T_A = e_T \Delta T_L + f_T \tag{34}$$

where a subscript T has been added to e and f We can also solve for

$$\Delta q_A = e_q \Delta T_L + f_q \tag{35}$$

The equation for e_q and f_q is the same as that for e and f, substituting the evaporation E for F. If the atmosphere uses a leapfrog time step we must once again remember to use $2\Delta t$ as the time step in these computations. Implciit atmospheric fluxes can be treated just as before. We can also define

$$\alpha_q \equiv E_0 + \frac{\partial E}{\partial q_A} f_q \tag{36}$$

$$\beta_q \equiv \frac{\partial E}{\partial T_L} + \frac{\partial E}{\partial q_A} e_q \tag{37}$$

The job of the surface model is unchanged – compute the change in surface temperature given a surface energy flux of the form:

$$\alpha + \beta \Delta T_L \tag{38}$$

The difference is that now the values passed to the surface model are

$$\alpha = \alpha_T + \alpha_q \tag{39}$$

and

$$\beta = \beta_T + \beta_q \tag{40}$$

5 Long wave radiation at the surface

In a climate model, there are radiative fluxes as well as fluxes of sensible and latent heat at the surface, which must be accounted for in the surface energy balance. Typically, short wave fluxes are treated explicitly, but the upward longwsave flux is treated implicitly, as it can be the dominant damping agent of surface temperature in some regions. The only changse in the equations that are required are the modifications to α and β resulting from the flux and its derivative with respect to surface temperature.

(There are issues here wtih regard to the fact the atmospheric radiative computation in FMS is explicit, and generates heating rates which are not modified when the surface modules determine ΔT_L and the correspondingly modified upward long wave flux. In effect, this modification to the long wave flux is assumed to pass through the atmosphere to space without absorption. A better assumption might be to absorb this modification to the flux in the lowest atmospheric layer?)

6 The exchange grid

Now suppose that the atmosphere and the land or ice models are on different grids. We define an exchange grid whose boundaries are determined by overlaying the boundaries of the atmosphere cells with those of the surface models. (See documentation of exchange grid module for further discussion of this exchange grid.) An atmospheric cell, or ice, land, or ocean cell, contains a finite set of exchange grid cells. As long as the flux is defined unambiguously on the exchange grid, and if the flux into an atmosphere or land surface cell is just the area-weighted mean over the exchange grid cells that it contains, then the fluxed quantity will be conserved.

Assume first that the fluxes are computed explicitly

$$\frac{c_A}{\Delta t}\Delta T_A = \overline{F}^A \tag{41}$$

$$\frac{c_L}{\Delta t}\Delta T_L = \overline{F}^L \tag{42}$$

The overlines refer to averages over the exchange cells within either the atmosphere or the surface cell

There are some problematic aspects of this interpolation scheme (which are unaffected by implicit corrections to these fluxes). Most relevant in this context is that the staggering of the grid and the resulting averaging results in artificial horizontal mixing. A disturbance initally localized at one grid cell on the surface will spread to other surface cells even though the exchanges in the unapproximated model are completely local.

If we now try to make the model fully implicit as before, we are in trouble because of this coupling. The flux sensitivities as well as the fluxes themselves must be defined on the exchange grid, and the equations would be

$$\frac{c_A}{\Delta t}\Delta T_A = \overline{F_0}^A + \overline{\frac{\partial F}{\partial T_A}}^A \Delta T_A + \overline{\frac{\partial F}{\partial T_L}\Delta T_L}^A \tag{43}$$

and

$$\frac{c_L}{\Delta t}\Delta T_L = \overline{F_0}^L + \overline{\frac{\partial F}{\partial T_A}\Delta T_A}^L + \overline{\frac{\partial F}{\partial T_L}}^L \Delta T_L \tag{44}$$

In general, all grid points in the atmosphere are now coupled with all points in the surface model(s). Solution would require iteration, which is a source of complexity that is totally inappropriate given that the underlying dynamics is purely local. As we have seen, explicit flux computation also generates artificial non-local coupling as a function of time – the fully implicit computation spreads the influence widely within one time step.

One straighforward alternative is to do everything related to the implicit time-stepping on the exchange grid, producing temperature and moisture increments defined on the exchange grid, and, as a last step, averaging these onto the grids of the respective models. One difficulty with this scheme is that in actual models the processes involved in the implicit computation of surface temperatures and fluxes can be rather complicated, and these parts of the models would have to compute on the exchange grid, whose dimensions can get quite large. It turns out that one can avoid doing the atmospheric diffusion computation on the exchange grid, but one still ends up with the surface component models split into a part computing on the exchange grid and a part on the model's own grid, in a way that causes considerable confusion. (An earlier version of our model was constructed in this way and rejected for these reasons.) It is preferable that the component models know nothing about the exchange grid.

While it is not clear that it is the ideal solution, the following scheme is the one currently implemented in FMS (Eugene). It treats the atmospheric side of the model differently from the surface compnent models (which we refer to as "land" here).

Fluxes and derivatives of fluxes are computed on the exchange grid. The flux is defined on the exchange grid to be

$$F_0 + \frac{\partial F}{\partial T_A}\Delta T_A^* + \frac{\partial F}{\partial T_L}\Delta T_L \tag{45}$$

where ΔT_A^*, computed as described below, varies across exchange cells within one atmospheric cell, while ΔT_L is uniform across the entire land cell.

Start as if one were computing the implicit temperature tendencies on the exchange grid and compute explicit fluxes and flux derivatives on the exchange grid. Continue by computing e and f (9) and then α and β (15) on the exchange grid. *Average α and β over the surface model grid.* Then instruct the surface model to use these averaged fluxes and derivatives to compute its new surface temperature implicitly. Copy this surface temperature increment to the exchange grid and then compute the atmospheric tendency in the lowest model level on the exchange grid. Average this atmospheric tendency over the atmospheric grid as the final step. The only distinction between this scheme and that in (43) is that the fluxes are consistent with the atnmospheric increments on the exchange grid (ΔT_A^*) before averaging, rather than with the final averaged increments.

7 Algorithm

Summarizing the final algorithm:

• We start with the state of all component models defined at time step i, or $i-1$ in the case of leapfrog models. The first step is to move everything that is needed to compute the surface fluxes onto the exchange grid. We then compute the explicit estimate of these fluxes on the exchange grid and all of the relevant derivatives. One must keep in mind that these flux values are temporary, and will be corrected by the implicit part of the computation, using these derivatives. This work is performed by a call to the subroutine *flux_calculation.*.

• Assume that the atmospheric model has computed the increment in the atmospheric temperature and specific humidity due to all terms treated explicitly (more precisely, all explicit terms that are included before the implicit vertical diffusion is applied.) From the myopic viewpoint of the surface exchange module, the only quantities of interest are the increments in temperature and specific humidity in the lowest atmospheric layer. If the model includes vertical diffusion, these increments include the effect of the explicit diffusive flux across the top of the lowest atmospheric layer If the vertical diffusion is implicit, then this increment must be computed with the modified flux (22) and one must also provide the "total" derivative (21), for both temperature and moisture. If there is no implicit flux across the top of the lowest atmospheric layer, then these derivatives must be set to zero.

• The surface exchange module assumes that the resulting increments and derivatives are packaged in a particular way within a data type defined and allocated within the atmospheric model. In addition to a variety of other field included in this type that are not involved in the implicit computation (such as precipitation or the net shortwave flux), five spatial fields of information are passed for this implicit algorithm: besides the increments of temperature and humidity in the lowest atmospheric layer, and the derivatives of the heat flux and the moisture flux at the top of this layer, the atmospheric time step ($2\Delta t$ for leapfrog) divided by the mass of the lowest atmospheric layer is also passed as part of this type.)

• Next, compute α_T, α_q, β_T, β_q on the exchange grid and average these onto the land and ice grids. This is performed by subroutine *flux_down_from_atmos*

• Assume that the land and ice models are now instructed to compute the new surface temperatures.

• Move the increments in surface temperature to the exchange grid, and compute the increment in the temperature and moisture of the lowest atmospheric layer. Also correct the surface sensible heat, evaporation, and long-wave radiation. Then average the increments of temperature and moisture in the lowest atmospehric layer onto the atmospheric grid. This is performed by subroutine *flux_up_to_atmos*

• Assume that the atmospheric model can now take these lowest layer increments and finalize the upward sweep of the tridiagonal elimination to complete the implicit computation of vertical diffusion.